

Spiro[furan-2(3H),1'(3'H)-isobenzofuran]-3,3'-dione

Other names:

4-phenyl-

Fluorescin

Fluorescamine

4-phenylspiro[furan-2(3H),1'(3'H)-isobenzofuran]-3,3'-dione

Inchi: InChI=1S/C17H10O4/c18-15-13(11-6-2-1-3-7-11)10-20-17(15)14-9-5-4-8-12(14)16(19)2

InchiKey: ZFKJVJIDPQDDFY-UHFFFAOYSA-N

Formula: C17H10O4

SMILES: O=C1OC2(OC=C(c3ccccc3)C2=O)c2ccccc21

Mol. weight [g/mol]: 278.26

CAS: 38183-12-9

Physical Properties

Property code	Value	Unit	Source
gf	21.98	kJ/mol	Joback Method
hf	-250.69	kJ/mol	Joback Method
hfus	30.09	kJ/mol	Joback Method
hvap	76.27	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	2.650		Crippen Method
mcvol	191.730	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	863.04	K	Joback Method
tc	1154.11	K	Joback Method
tf	610.07	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.64	J/molxK	863.04	Joback Method
cpg	591.94	J/molxK	911.55	Joback Method
cpg	607.96	J/molxK	960.06	Joback Method
cpg	624.03	J/molxK	1008.58	Joback Method
cpg	640.43	J/molxK	1057.09	Joback Method
cpg	657.48	J/molxK	1105.60	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38183129&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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